❖ Carboranes

Carboranes are the cluster composed of carbon, boron and hydrogen atoms; and just like boranes, can be classified as closo-, nido-, arachno-, hypho-, or -klado based on whether they represent a complete (closo) polyhedron, or a polyhedron that is missing one (nido-), two (arachno-), or more vertices. Carboranes are the most common examples of heteroboranes. The electronic structure of carboranes has been described by Wade-Mingos rules. Three main categories of carboranes are discussed below.

➢ *Closo-(Closed) Carboranes*

These are closed triangular polyhedral structures in which all the vertices of the triangular polyhedral geometries are occupied mainly by boron and some sites by carbon atoms. There are n+1 electron pairs (or 4n+2 skeletal electrons) involved in multicentre bonding in closo-carborane; where n represents the total number of B and C atoms. Some of the common examples of closo-carboranes are:

1. $C_2B_{10}H_{12}$: In $C_2B_{10}H_{12}$, n = 12; according to Wade's rule, the two CH units contribute 2×3 = 6 electrons and ten BH units contribute 10×2 = 20 electrons to the bonding molecular orbitals or to the skeletal structure. Thus, there are 13 electron pairs (n+1 = 13) present in the multicentre bonding orbitals of $C_2B_{10}H_{12}$, confirming this as a closo kind. Three isomers (ortho-, meta- and para-) are possible.

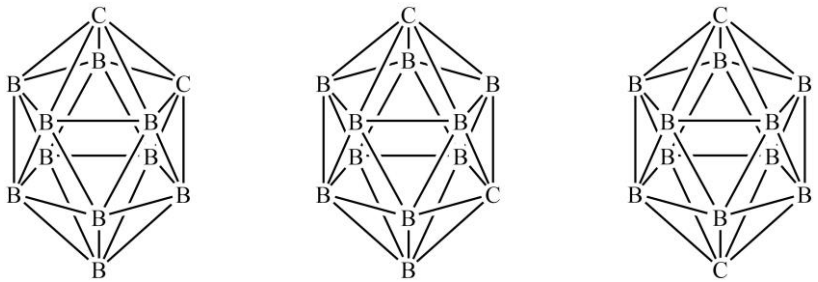


Figure 19. Structure and isomerism in $C_2B_{10}H_{12}$ (dicarba-closo-dodecaborane).

2. $C_2B_3H_5$: In $C_2B_3H_5$, n = 5; according to Wade's rule, the two CH units contribute 2×3 = 6 electrons and three BH units contribute 3×2 = 6 electrons to the bonding molecular orbitals or the skeletal structure. Thus there are 6 electron pairs (n+1 = 6) present in the multicentre bonding orbitals of $C_2B_3H_5$, confirming this as closo kind. Three isomers are possible which are given below.

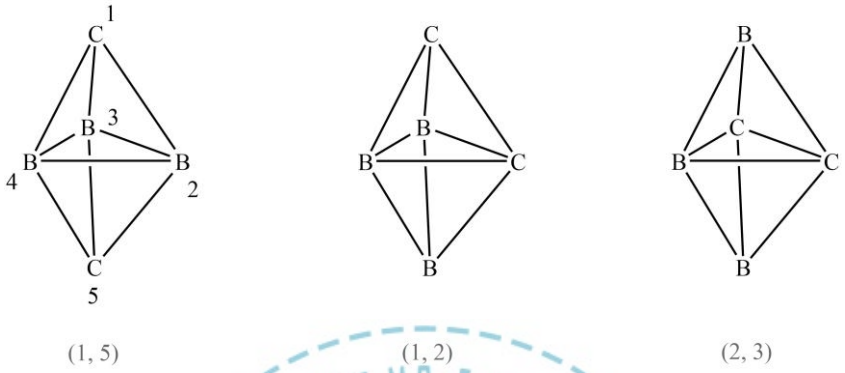


Figure 20. Structure and isomerism in $C_2B_3H_5$.

➢ ***Nido-(Nestlike) Carboranes***

These are nest-like geometries and can be assumed as the derivatives of closed triangular polyhedral structures in which one vertex is removed. Most of the sites in these clusters are occupied by boron atoms while some sites by carbons. There are n+2 electron pairs (or 4n+4 skeletal electrons) involved in multicentre bonding in nido-carboranes; where n represents the total number of B and C atoms. Common examples are:

1. $C_2B_9H_{13}$: In $C_2B_9H_{13}$, n = 11; and according to Wade's rule, the two CH units contribute 2×3 = 6 electrons, nine BH units contribute 9×2 = 18 electrons, and two additional hydrogens contribute 2×1 = 2 electrons to the bonding molecular orbitals or the skeletal structure. Thus there are total 26 electrons or 13 electron pairs (n+2 = 13) present in the multicentre bonding orbitals of $C_2B_9H_{13}$, confirming this as nido kind. The structure of some of the possible isomers that can be obtained experimentally are given below.

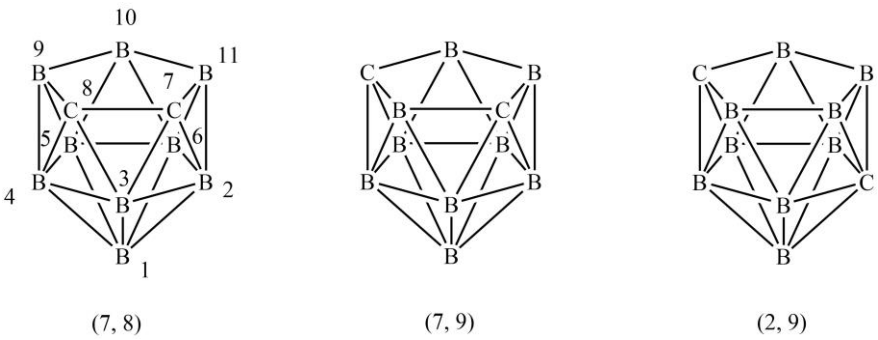
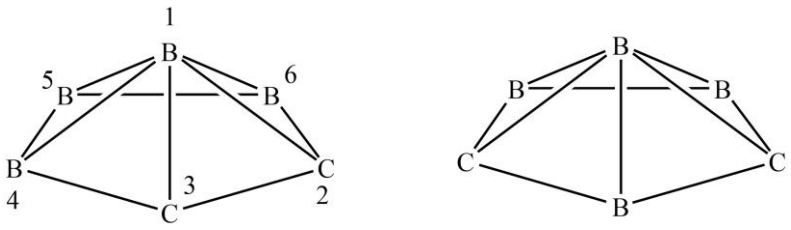


Figure 21. Structure and isomerism in $C_2B_9H_{13}$.

2. $C_2B_4H_8$: In $C_2B_4H_8$, n = 6; according to Wade's rule, the two CH units contribute 2×3 = 6 electrons and three BH units contribute 4×2 = 8 electrons and two additional hydrogens contribute 2×1 = 2 electrons to the bonding molecular orbitals or the skeletal structure. Thus there are total 16 electrons or 8 electron pairs (n+2 = 8) present in the multicentre bonding orbitals of $C_2B_4H_8$, confirming this as a nido kind. The structure of some of the possible isomers that can be obtained experimentally are given below.



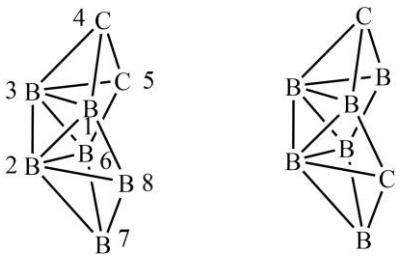
(2, 3) (2, 4)

Figure 22. Structure and isomerism in $C_2B_4H_8$.

➢ ***Arachno-(Weblike) Carboranes***

These are web-like geometries and can be assumed as the derivatives of closed triangular polyhedral structures in which two vertices are removed. Most of the sites in these clusters are occupied by boron atoms while some sites by carbons. There are n+3 electron pairs (or 4n+6 skeletal electrons) involved in multicentre bonding in arachno-carboranes; where n represents the total number of B and C atoms. Some of the common examples of arachno-carboranes are:

1. $C_2B_6H_{12}$: In $C_2B_6H_{12}$, n = 8; according to Wade's rule, the two CH units contribute 2×3 = 6 electrons and six BH units contribute 6×2 = 12 electrons and four additional hydrogens contribute 4×1 = 4 electrons to the bonding molecular orbitals or the skeletal structure. Thus there are total 22 electrons or 11 electron pairs (n+3 = 11) present in the multicentre bonding orbitals of $C_2B_6H_{12}$, confirming this as an arachno kind. The structure of some of the possible isomers that can be obtained experimentally are given below.



(4, 5) (4, 8)

Figure 23. Structure and isomerism in $C_2B_6H_{12}$.

2. $C_2B_7H_{13}$: In $C_2B_7H_{13}$, $n = 9$; according to Wade's rule, the two CH units contribute $2\times3 = 6$ electrons and seven BH units contribute $7\times2 = 14$ electrons and four additional hydrogens contribute $4\times1 = 4$ electrons to the bonding molecular orbitals or the skeletal structure. Thus there are total 24 electrons or 12 electron pairs (n+3 = 12) present in the multicentre bonding orbitals of $C_2B_7H_{13}$, confirming this as an arachno-kind. The structure of some the possible isomers that can be obtained experimentally are given below.

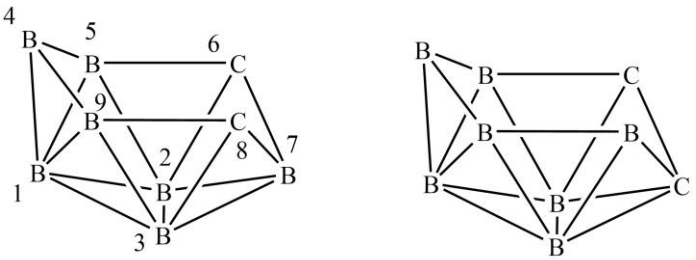


Figure 24. Structure and isomerism in $C_2B_7H_{13}$.

➢ ***Structural Pattern Correlation Between Closo, Nido and Arachno Carboranes***

The structural pattern in closo, nido and arachno carboranes for different vertexes and skeletal electron pairs is very much important to to theoretical as well experimental analysis. Hs are omitted for clarity.

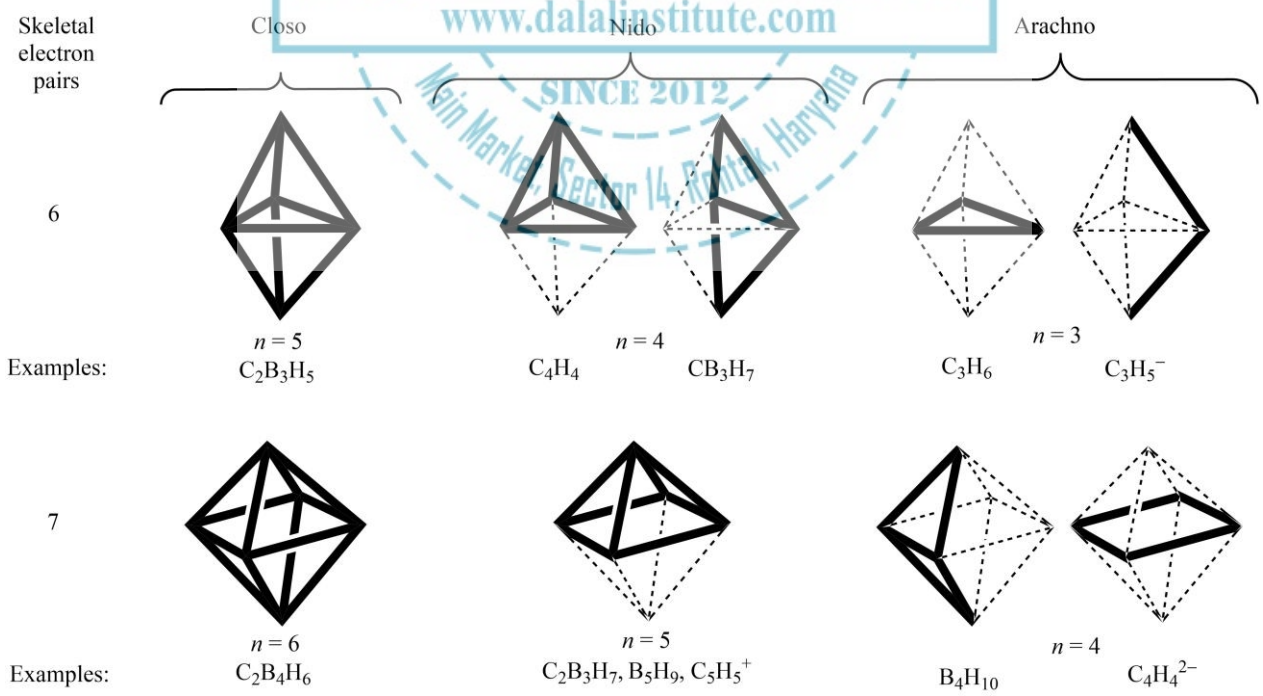
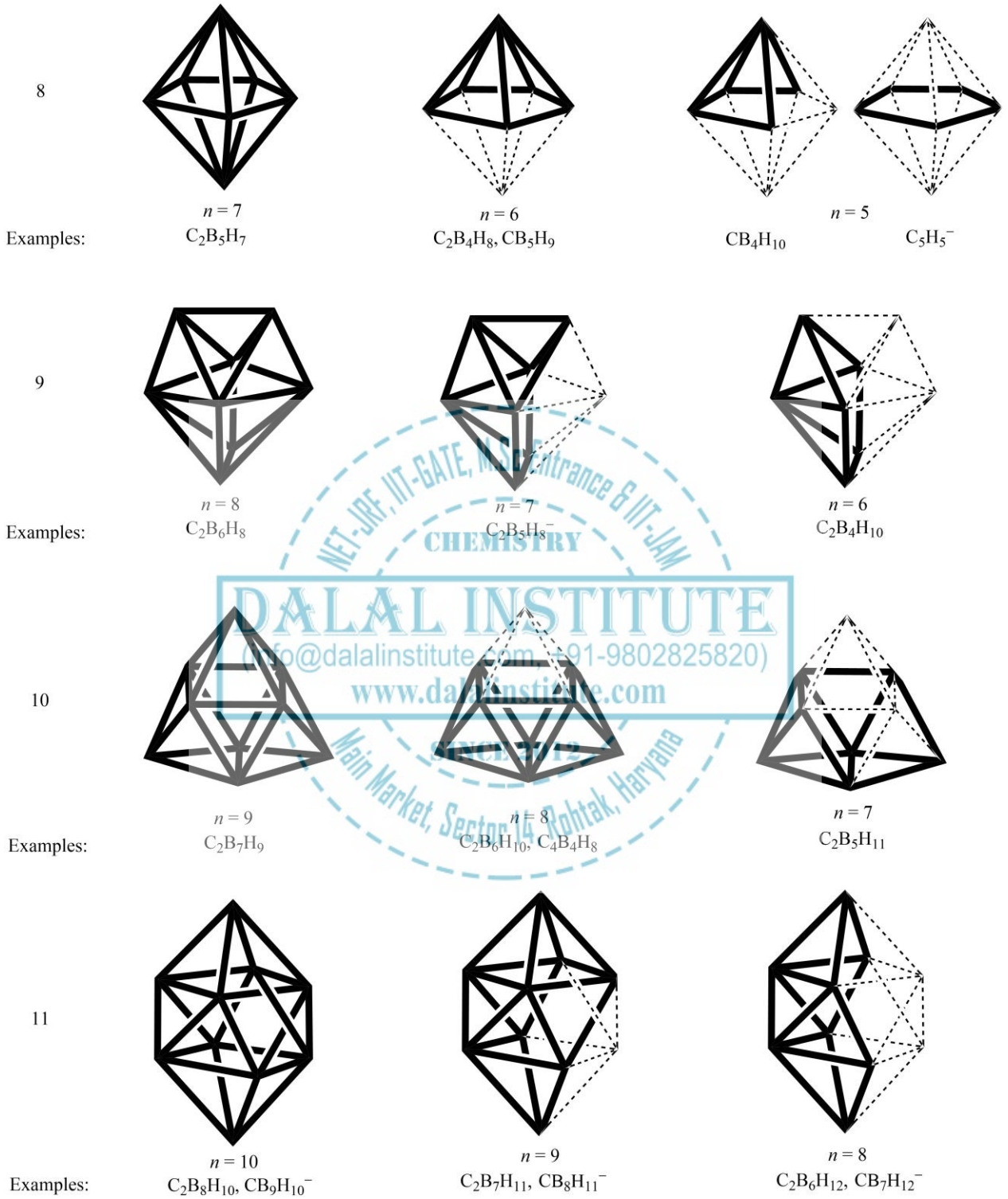


Figure 25. Continued on the next page…



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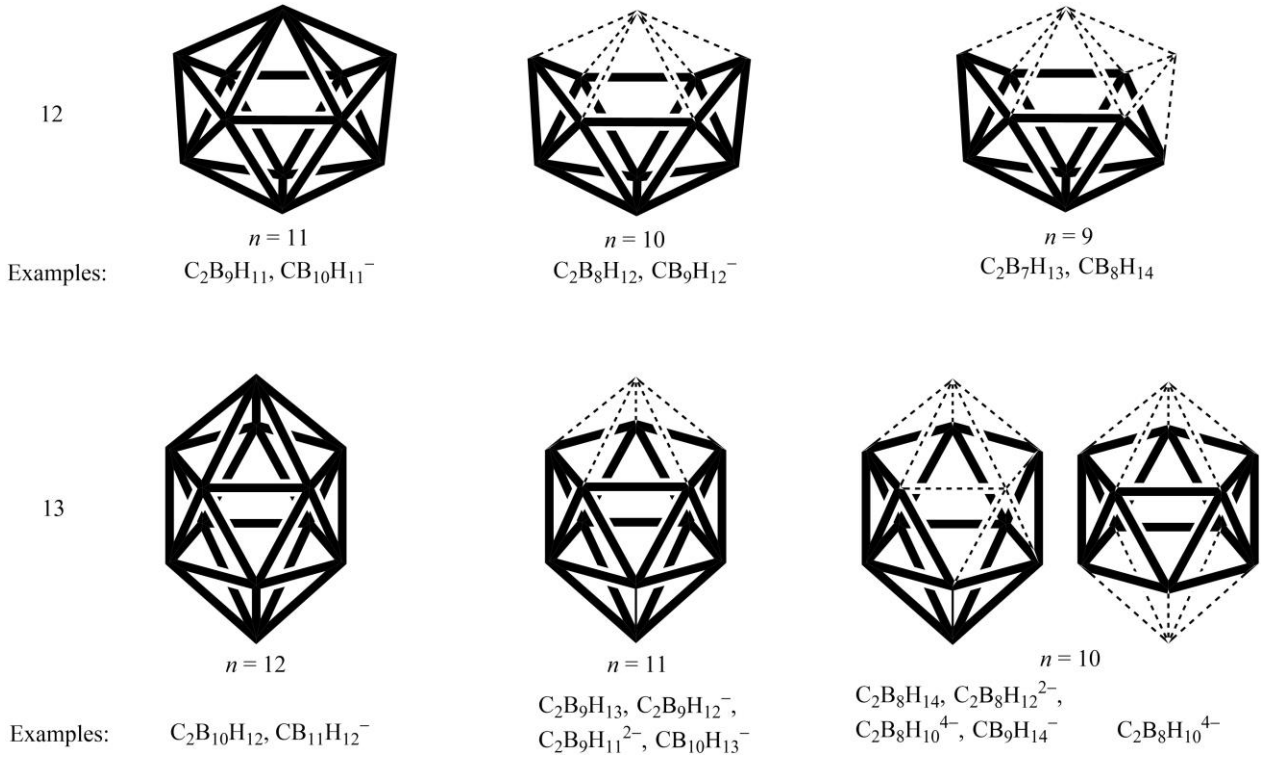

Figure 25. The structural relationship between closo, nido, and arachno carboranes.

Some hypho-carboranes ($C_2B_{n-2}H_{n+6}$) also do exist in which three vertices from the parent deltahedron are missing. Furthermore, carboranes are also formed by joining two or more preceding types; called as conjuncto-carboranes.

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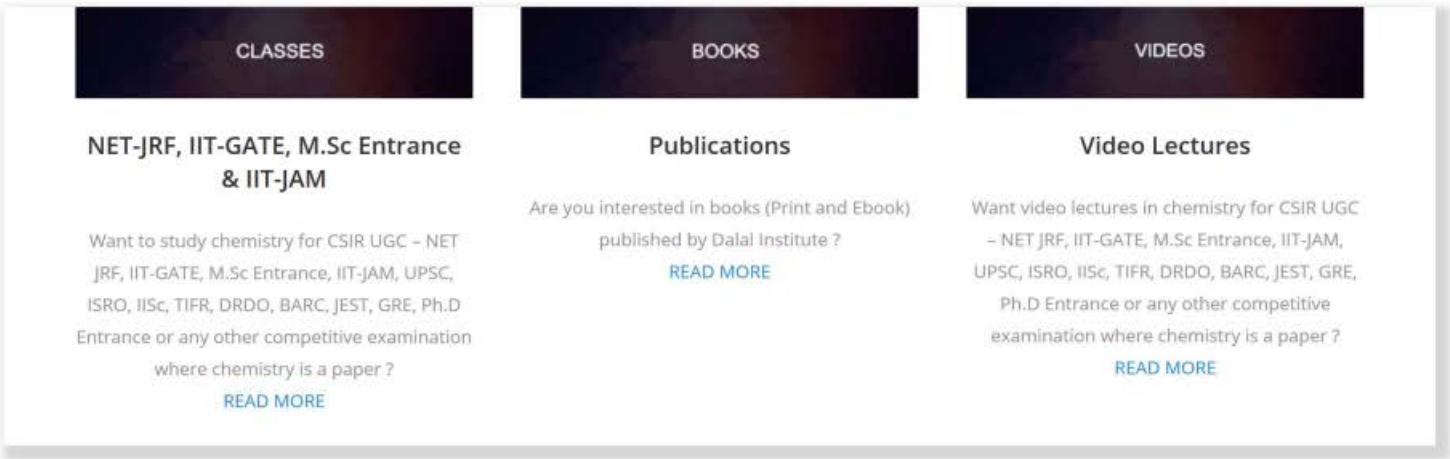

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